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LLNL-TR-672399

An Anonymous Referee Report

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June 8, 2015

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Ms. ID: ac-2015-016992, Analytical Chemistry

Title: Sensitivity to actinide doping of uranium compounds by resonant inelastic x-ray scattering at U L3 edge

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This is a combined experimental and theoretical study of the compound UO_2 , $\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_6$ and $\text{UO}_{0.75}\text{Pu}_{0.25}\text{O}_2$, using resonant inelastic x-ray scattering (RXIS), high resolution x-ray absorption (XAS) and LDA and LDA-U calculations. The higher resolution of the measurements permits the observation of changes that were previously unresolvable. This is an excellent piece of work and should be published in AC. However, there are some significant issues that need to be addressed and mandatory changes are required. Here are some specifics, not necessarily in the order of importance.

1. The English needs to be improved. There are places throughout where articles such as “a, an, & the” are missing.
2. The authors need to reference and discuss the prior results by Corwin Booth et al in PNAS 2012 and JESRP 2014. In particular, the high resolution L_3 XANES and extracted 6d DOS's (including UO_2) should be compared to the present work.
3. Page 4: Was there no triple containment for the Pu sample? A kapton film may be sufficient for U materials but what about Pu?
4. Page 5: scalar relativistic (no spin orbit) calculations. This needs to be justified. Experimental results with 5d XAS/EELS and atomic calculations (Gerrit van der Laan et al, PRL 2004) and LDA calculations by Andrey Kutepov (PRB 2005) indicate a large spin orbit splitting in the 5f's, on the order of 1 to 2 eV.
5. Page 12: Figure 3. The contour plots are very pretty but individual plots are needed to properly assess the level of agreement between experiment and theory.